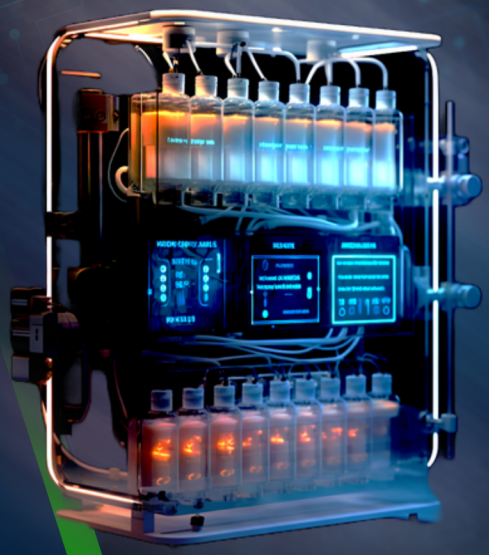
SimulationsPlus

GastroPlus

OPT

OPTIMIZATION

The Optimization Module performs the multidimensional search needed to fit model parameters to one or more data sets automatically. Objective function weighting is user-defined, and includes the most common weighting schemes.



Fitting Models to Data

One of the most important uses of GastroPlus® is to fit absorption, pharmacokinetic, and pharmacodynamic models to observations. In doing so, researchers gain tremendous insight into how their compound is behaving *in vivo*. When a single set of model parameters can be found that properly describes the observed plasma concentration vs. time profiles for all dose levels, a useful model has been obtained. In general, if the model parameters must be changed for each dose level, then something is not being accounted for correctly.

Example Parameters:

- PBPK model parameters to plasma and/or tissue concentration vs. time data
- Peff and absorption scale factors to determine regional dependencies
- A wide variety of physiological parameters (when necessary – rarely used)
- Parameters to match profiles of parent drugs or any of their metabolites

What is the Optimization module?

The Optimization Module for GastroPlus extends and enhances the program's basic capabilities in several important ways:

- To automatically fit physiochemical, pharmacokinetic, formulation and/or physiology model parameters to data
- To optimize study designs (e.g., dosing regimens)
- To "deconvolute" *in vivo* release profiles to achieve a target plasma (or tissue) concentration vs. time curves for parent and/or metabolites

Flexible optimization settings

Optimization with multiple drug records, multiple objective functions, and multiple observed data like concentration profile, C_{max}, T_{max}, and AUC.

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Interested in collaborating?

Email us! info@simulations-plus.com

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